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On the deterministic computation of functional integrals in application to quantum mechanical problems

M. GREGUŠ, Jr. *, Yu.Yu. LOBANOV, O.V. SIDOROVA and E.P. ZHIDKOV
Laboratory of Computing Techniques and Automation, Joint Institute for Nuclear Research, Dubna, U.S.S.R.

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Abstract: New approximate formulae for functional integrals with Gaussian measure in separable Frechét spaces are derived. As a special case, the integration with respect to the conditional Wiener measure is investigated. For conditional Wiener integrals a family of approximate formulae with weight is constructed. The quantum mechanical models, namely the linear and the inharmonic oscillators, are described. The efficiency of the formulas is demonstrated in the numerical comparison with the Monte Carlo method on lattice.

Keywords: Functional integral, quantum mechanics, Frechét space, Gaussian measure, conditional Wiener measure, linear oscillator, anharmonic oscillator, approximate formula, numerical integration.

§ 1

One of the most effective mathematical techniques in the contemporary quantum field theory is the method of functional integration (e.g. [6]). One of its great successes is the development of the lattice gauge theory. Introduction of a space–time lattice turns functional integrals into ordinary ones of high dimension ($\gtrsim 10^5$) that are usually evaluated by the Monte Carlo method on powerful computers. Recently, works have appeared ([2], see also [6]) presenting the ways of computation of functional integrals that do not need the lattice-discretization methods. In the latter sense, the approach based on the mathematically rigorous study of functional integrals with respect to Gaussian measure [4,5] seems to be promising. In the present paper, we derive, within the framework of the mentioned approach, several new approximation formulae for functional integrals which are exact on a class of polynomial functionals of a given degree. Using these formulae we compute certain characteristics in Euclidean quantum mechanics. On the models of the linear quantum oscillator and of the inharmonic oscillator, we compare our results with the results of computations of functional integrals that have been obtained, in [2], via the approximation of paths in the functional, and also, in [3] and [12], by the Monte Carlo method

* Permanent address: Matematicko-fyzikálna fakulta, Univerzita Komenského, Bratislava, Czechoslovakia.

on lattice. The employment of the derived approximation formulae replaces the evaluation of the considered functional integral by the evaluation of an ordinary integral of a low dimension, thus allowing the use of the deterministic methods (Gaussian quadrature, Tchebyshev, etc.) and leading to a significant economy of computer time and memory. The comparison of numerical results confirms the higher efficiency of the method employed.

§ 2

We shall study a functional integral $\int_Y F[x]\,\mathrm{d}\mu(x)$, where $F[x]$ is a real functional defined on a separable Frechét space Y. $\mu(x)$ is a Gaussian measure defined on Y by a correlation functional $K(\xi, \eta)$ and by a mean value $m(\xi)$, $x \in Y$, $\xi, \eta \in Y'$. Let H be a Hilbert space generated by the measure μ with a scalar product $(\cdot, \cdot)$ and an orthonormal basis $\{e_i\}$, $i = 1, 2, 3, \ldots$. Under certain conditions on a function $\rho(r)$: $R \to Y$ [7] we can prove the following theorem.

Theorem 1. *Suppose*

$$S_n(x) = \sum_{k=1}^{n} (e_k, x)e_k; \qquad U_n(u) = \sum_{k=1}^{u} u_k e_k, \quad u \in \mathbb{R}^n;$$

$$\theta_m(v) = \sum_{k=1}^{m} c_{m,k}\rho(v_k), \quad v \in \mathbb{R}^m;$$

$[c_{m,k}]^2$, $k = 1, 2, \ldots, m$, *are the roots of*

$$Q_m(r) = \sum_{k=0}^{m} (-1)^k r^{m-k}/k!.$$

Then the following 'composite approximation formula':

$$\int_Y F[x]\,\mathrm{d}\mu(x)$$

$$= (2\pi)^{-n/2} \int_{\mathbb{R}^n} \exp\{-(u, u)/2\} \int_{\mathbb{R}^m} F\left[\theta_m(v) - \theta_{m,n}(v) + U_n(u)\right] \mathrm{d}\nu^m(v)\,\mathrm{d}u$$

$$+ R_{m,n}(F), \tag{1}$$

is exact for all polynomial functionals of degree $\leqslant 2m + 1$. *Here* $\theta_{m,n}(v) = S_n(\theta_m(v))$ *and the measure* ν^m *in* $\mathbb{R}^m$ *is a cartesian product of symmetric probabilistic measures* ν *in* $\mathbb{R}$.

Remark. The proof of Theorem 1 and of the convergence of the remainder $R_{m,n}(F)$ to zero, and, moreover, the estimate of $R_{m,n}(F)$ are given in [7].

Practical example. We consider an integral with a conditional Wiener measure $\mathrm{d}_w\check{}x$ ($Y = \{C[0, 1];\ x(0) = x(1) = 0\} = C$, mean value $m(r) = 0$, correlation function $B(r, s) = \min\{r, s\}$

$-rs$). Then we obtain a special case of (1):

$$\int_C F[x]\, \mathrm{d}_{\mathrm{w}}{}^{\vee}x = (2\pi)^{-n/2} \int_{\mathbb{R}^n} \exp\{-\tfrac{1}{2}(u, u)\} 2^{-m} \times \underbrace{\int_{-1}^{1} \cdots \int_{-1}^{1}}_{m} F\left[\tilde{\theta}_m(v, \cdot) - \tilde{\theta}_{m,n}(v, \cdot) + \tilde{U}_n(u, \cdot)\right] \mathrm{d}v\, \mathrm{d}u + R_{m,n}(F), \tag{2}$$

$$\tilde{\theta}_m(v, t) = \sum_{k=1}^{m} c_{m,k} \tilde{\rho}(v_k, t); \qquad \tilde{\rho}(r, t) = \begin{cases} -t\,\mathrm{sign}(r), & t \leqslant |r|, \\ (1-t)\,\mathrm{sign}(r), & t > |r|; \end{cases}$$

$$\tilde{U}_n(u, t) = \sum_{k=1}^{n} \frac{\sqrt{2}}{k\pi} u_k \sin(k\pi t);$$

$$\tilde{\theta}_{m,n}(v, t) = \sum_{k=1}^{n} \frac{2}{k\pi} \sin(k\pi t) \sum_{j=1}^{m} c_{m,j}\, \mathrm{sign}(v_j) \cos(k\pi v_j).$$

We have used (2) in our computations. Therefore we have investigated its properties. For instance, its order of convergence equals to $O(n^{-m-1})$.

§ 3

Here we shall study a significant to quantum mechanics case of Gaussian measure i.e. the conditional Wiener measure $\mathrm{d}_{\mathrm{w}}{}^{\vee}x$.

In constructing the approximation formulae for

$$I(P \cdot F) = \int_C P[x] F[x]\, \mathrm{d}_{\mathrm{w}}{}^{\vee}x \tag{3}$$

with weight

$$P[x] = \exp\left\{\int_0^1 \left[\lambda p(t) x^2(t) + g(t) x(t)\right] \mathrm{d}t\right\}, \tag{4}$$

$\lambda \in \mathbb{R}$; $p(t)$, $g(t) \in C[0, 1]$, our next theorem plays an important rôle.

Theorem 2 [8]. *The integral* (3) *with weight* (4) *can be written in the form*

$$I(P \cdot F) = \exp\left\{-\tfrac{1}{2}\int_0^1 (1-s) K(s)\, \mathrm{d}s\right\} \exp\left\{\tfrac{1}{2}\int_0^1 L^2(t)\, \mathrm{d}t\right\} \int_C F[\phi(x) + a]\, \mathrm{d}_{\mathrm{w}}{}^{\vee}x,$$

where

$$\phi(x(t)) = x(t) - \frac{1-t}{V(t)} \int_0^t K(s) V(s) x(s)\, \mathrm{d}s, \qquad V(t) = \exp\left\{\int_0^t (1-s) K(s)\, \mathrm{d}s\right\},$$

$K(s)$ *is a solution of the differential equation*

$$(1-s)K'(s) - (1-s)^2 K^2(s) - 3K(s) - 2\lambda p(s) = 0, \quad s \in [0, 1],$$

with initial condition $K(1) = -\frac{2}{3}\lambda p(1)$,

$$a(t) = \int_0^t L(s)\,\mathrm{d}s - \frac{1-t}{V(t)}\int_0^t K(s)V(s)\left[\int_0^s L(u)\,\mathrm{d}u\right]\mathrm{d}s,$$

$$L(t) = \int_0^t \left[K(s)V(s)H(s) - g(s)\right]\mathrm{d}s + c, \qquad H(t) = \int_t^1 g(s)\frac{1-s}{V(s)}\mathrm{d}s,$$

and the constant c *is determined by the condition*

$$\int_0^1 L(s)\,\mathrm{d}s = 0.$$

Theor [8]. *Under the conditions of the above theorem the approximation formula*

$$\int_C \exp\left\{\int_0^1 \left[\lambda p(t)x^2(t) + g(t)x(t)\right]\mathrm{d}t\right\}F[x]\,\mathrm{d}_{\mathrm{w}}{}^{\vee}x$$

$$\approx \exp\left\{-\tfrac{1}{2}\int_0^1 (1-s)K(s)\,\mathrm{d}s\right\}\exp\left\{\tfrac{1}{2}\int_0^1 L^2(t)\,\mathrm{d}t\right\}$$

$$\times 2^{-m}\int_{-1}^1 \cdots \int_{-1}^1 F\left[\tilde{\Psi}_m(v,\cdot) + a(\cdot)\right]\mathrm{d}v_1 \cdots \mathrm{d}v_m, \tag{5}$$

is exact for every polynomial functional of degree $\leqslant 2m+1$. *Here*

$$\tilde{\Psi}_m(v,\cdot) = \sum_{k=1}^m c_{m,k}\tilde{\sigma}(v_k,\cdot), \qquad \tilde{\sigma}(r,\cdot) = \phi(\tilde{\rho}(r,\cdot)) = \tilde{f}(r,\cdot) - \tilde{\kappa}(r,\cdot),$$

$$\tilde{\kappa}(r,t) = \begin{cases} \operatorname{sign}(r), & t \leqslant |r|, \\ 0, & t > |r|, \end{cases}$$

$$\tilde{f}(r,t) = \operatorname{sign}(r)\frac{1-t}{V(t)}\left[1 + \int_0^{\min\{|r|,t\}} K(s)V(s)\,\mathrm{d}s\right.$$

Remark [9]. In the proof of Theorem 3 we employ the transformation $x(t) \mapsto y(t)$ defined by the relation

$$y(t) = x(t) + (1-t)\int_0^t K(s)x(s)\,\mathrm{d}s, \qquad K(s) \in C[0,1].$$

This transformation maps the space C onto itself in one-to-one correspondence. The inverse transformation $\phi(y(t))$: $y(t) \mapsto x(t)$ is given by the relation

$$x(t) = y(t) - (1-t)\exp\left\{-\int_0^t (1-s)K(s)\,\mathrm{d}s\right\}$$

$$\times \int_0^t \exp\left\{\int_0^s (1-u)K(u)\,\mathrm{d}u\right\}K(s)y(s)\,\mathrm{d}s.$$

Now we will study, in more detail, one particular case of the formula (5). If we set $p(t) \equiv 1$, $g(t) = g = \text{const.}$, $\lambda < \frac{1}{2}\pi^2$, then (5) acquires the form

$$I(P \cdot F) = \int_C \exp\left\{\int_0^1 \left[\lambda x^2(t) + g x(t)\right] \mathrm{d}t\right\} F[x] \, \mathrm{d}_w x \approx I_m(P \cdot F)$$

$$= \sqrt{\frac{\sqrt{2\lambda}}{\sin\sqrt{2\lambda}}} \exp\left\{\frac{g^2}{2\lambda\sqrt{2\lambda}}\left[\tan\sqrt{\tfrac{1}{2}\lambda} - \sqrt{\tfrac{1}{2}\lambda}\right]\right\} 2^{-m}$$

$$\times \int_{-1}^1 \cdots \int_{-1}^1 F\left[\tilde{\Psi}_m(v, \cdot) + a(\cdot)\right] \mathrm{d}v_1 \cdots \mathrm{d}v_m. \tag{6}$$

In this case $a(t)$ can be expressed explicitly as

$$a(t) = g\left(\lambda \cos\sqrt{\tfrac{1}{2}\lambda}\right)^{-1} \sin\sqrt{\tfrac{1}{2}\lambda}\, t \, \sin\sqrt{\tfrac{1}{2}\lambda}\,(1-t)$$

that may be useful in actual application of (6).

The transformation $\phi(x)$ acquires a simple form, too:

$$\phi(x) = x - \Phi(x) \tag{7}$$

where

$$\Phi(x(t)) = \sin\sqrt{2\lambda}\,(1-t) \int_0^t f(s) x(s) \, \mathrm{d}s,$$

and

$$f(s) = \frac{\sqrt{2\lambda}\,(1-s)\cos\sqrt{2\lambda}\,(1-s) - \sin\sqrt{2\lambda}\,(1-s)}{(1-s)\sin^2\sqrt{2\lambda}\,(1-s)}.$$

To estimate the remainder $R_m(P \cdot F) = I(P \cdot F) - I_m(P \cdot F)$ we need the following lemma.

Lemma. *Linear operator ϕ, defined on C according to* (7), *is bounded on C in L_2-norm.*

Proof. The parallelogram law in L_2-norm $\| \cdot \|$ yields

$$\| \phi(x) \|^2 \leqslant 2 \| x \|^2 + 2 \| \Phi(x) \|^2.$$

After some calculation it can be shown that $\| \Phi(x) \|^2 \leqslant \int_0^1 x^2(s) \omega(s) \, \mathrm{d}s$,

where $\omega(s) = f^2(s) \frac{1}{2}\left(1 - s - \dfrac{\sin 2\sqrt{2\lambda}\,(1-s)}{2\sqrt{2\lambda}}\right)$.

To estimate $\omega(s)$ we use the substitution $\tau = \tau(s) = \sqrt{2\lambda}\,(1-s)$. For $0 \leqslant s \leqslant 1$ we have $\tau \leqslant \sqrt{2\lambda}$ and $\tau/\sin\tau \leqslant \sqrt{2\lambda}/\sin\sqrt{2\lambda} = \tau_0$. Hence we obtain the estimate: $|\omega(s)| \leqslant \frac{1}{3}\tau_0^2 \lambda^2 (\frac{1}{3}\tau_0 + 1)^2 = \frac{1}{2}\omega_0$. Therefore the inequality $\| \phi(x) \|^2 \leqslant \alpha \| x \|^2$, $\alpha = 2 + \omega_0$, holds for all $x(t) \in C$. Thus the proof of the lemma is complete. □

Theorem 4. *Suppose the functional $F[x]$ can be expressed in the form*

$$F[x] = P_{2m+1}[x] + r_{2m+1}[x],$$

$P_{2m+1}[x]$ is a polynomial functional of a degree $\leqslant 2m+1$, and

$$|r_{2m+1}[x]| \leqslant c_1(m) \exp\left\{c_2(m) \int_0^1 x^2(t) \, \mathrm{d}t\right\}, \quad \text{with } c_1(m),\ c_2(m) \geqslant 0,$$

$0 \leqslant \lambda + c_2(m) < \frac{1}{2}\pi^2$. *Then there holds the estimate*

$$|R_m(P \cdot F) \leqslant c_1(m)\{A(m)M(g, \lambda)[\tfrac{8}{3}\exp(\tfrac{2}{3}c_2(m))]^m + M(g, \lambda + c_2(m))\},$$

where

$$A(m) = \exp\left\{2c_2(m)\int_0^1 a^2(t)\,dt\right\} = \exp\left\{\frac{c_2(m)g^2}{\lambda^2\cos^2\sqrt{\frac{1}{2}\lambda}}\left(2 + \cos\sqrt{2\lambda} - 5\frac{\sin\sqrt{2\lambda}}{\sqrt{2\lambda}}\right)\right\},$$

$$M(g, \lambda) = \int_C F[x]\,d_w x = \sqrt{\frac{\sqrt{2\lambda}}{\sin\sqrt{2\lambda}}}\exp\left\{\frac{g^2}{2\lambda\sqrt{2\lambda}}\left[\tan\sqrt{\tfrac{1}{2}\lambda} - \sqrt{\tfrac{1}{2}\lambda}\right]\right\}.$$

Proof. Since the formula (5) is exact for $P_{2m+1}[x]$, it follows that

$$|R_m(P \cdot F)| = |R(P \cdot r_{2m+1})| \leqslant |I(P \cdot r_{2m+1})| + |I_m(P \cdot r_{2m+1})|,$$

where

$$|I(P \cdot r_{2m+1})| \leqslant c_1(m)M(g, \lambda + c_2(m)),$$

and

$$|I_m(P \cdot r_{2m+1})| \leqslant c_1(m)M(g, \lambda)2^{-m} \times \int_{-1}^1 \cdots \int_{-1}^1 \exp\left\{c_2(m)\int_0^1 [\phi(\tilde{\theta}_m(v, t)) + a(t)]^2\,dt\right\} dv.$$

Using our lemma we get the inequality

$$\exp\left\{c_2(m)\int_0^1 [\phi(\tilde{\theta}_m(v, t)) + a(t)]^2\,dt\right\} \leqslant A(m)\exp\left\{2c_2(m)\alpha\int_0^1 \tilde{\theta}_m^2(v, t)\,dt\right\}.$$

Applying the Cauchy–Bunyakovskii inequality and the property that $\sum_{k=1}^m c_{m,k}^2 = 1$, we obtain

$$\tilde{\theta}_m^2(v, t) = \left[\sum_{k=1}^m c_{m,k}\tilde{\rho}(v_k, t)\right]^2 \leqslant \sum_{k=1}^m \tilde{\rho}^2(v_k, t).$$

Since $\int_0^1 \tilde{\rho}^2(v_k, t)\,dt = v_k^2 - |v_k| + \frac{1}{3}$, there follows (here we denote $u^2 - u + \frac{1}{3} = q(u)$, $u \in \mathbb{R}$) the inequality

$$|I_m(P \cdot r_{2m+1})| \leqslant c_1(m)M(g, \lambda)A(m)\left[2\int_0^{1/2}\exp\{2c_2(m)\alpha q(u)\}\,du\right]^m.$$

Employing the convexity of exponential function we get

$$\int_0^{1/2}\exp\{2c_2(m)\alpha_q(u)\}\,du \leqslant 2(\tfrac{4}{3}\exp\tfrac{2}{3}\alpha c_2(m) - \exp\tfrac{1}{6}\alpha c_2(m)) \leqslant \tfrac{8}{3}\exp\{\tfrac{2}{3}\alpha c_2(m)\}.$$

Therefore

$$|I_m(P \cdot r_{2m+1})| \leqslant c_1(m)M(g, \lambda)A(m)[\tfrac{8}{3}\exp(\tfrac{2}{3}\alpha c_2(m))]^m. \quad \square$$

§ 4

In this section we illustrate the use of the formulae with examples of simple quantum-mechanical models characterized by the Hamiltonian $H = \frac{1}{2}p^2 + V(X)$, $X \in (-\infty, \infty)$. We investigate

Table 1

T	Form. (6)		n	Form. (2)	CPU (s)
	$E_0^{(T)}$	$\lvert\psi_0^{(T)}(X)\rvert^2$		$E_0^{(T,n)}$	
5	0.50678	$1.0345\frac{1}{\sqrt{\pi}}\exp(-0.9866X^2)$	1	0.5077	1.8
6	0.50248	$1.0150\frac{1}{\sqrt{\pi}}\exp(-0.9951X^2)$	2	0.5073	3.1
7	0.50091	$1.0064\frac{1}{\sqrt{\pi}}\exp(-0.9982X^2)$	3	0.5010	5.5
8	0.50034	$1.0027\frac{1}{\sqrt{\pi}}\exp(-0.9993X^2)$	5	0.5002	9.7

the energy E_0 of the ground state and the energy $E_1 = E_0 + \Delta E$ of the first excited state of a system, the propagator $G(\tau)$ and the wave function $\psi_0(X)$ of the ground state (here characterized by the value $|\psi_0(X)|^2$). The basis for the evaluation of these quantities is the Green function $\langle X|e^{-HT}|X\rangle = \tilde{Z}(X, T)$, that has been expressed in the form of a functional integral with respect to the conditional Wiener measure in the following way [10]:

$$\tilde{Z}(X, T) = \frac{1}{\sqrt{2\pi T}} \int_C \exp\left\{ -T\int_0^1 V\left(\sqrt{Tx}\,(t) + X\right) dt \right\} d_w{}^{\vee}x. \tag{8}$$

(For the sake of brevity we do not list the other formulae.)

Consider the case of harmonic oscillator. Then the functional integral (8) with $V(X) = \frac{1}{2}X^2$ may be given explicitly using (6),

$$\tilde{Z}(X, T) = \frac{1}{\sqrt{2\pi \operatorname{sh} T}} \exp\{-\operatorname{th} \tfrac{1}{2}TX^2\}.$$

For finite T, similarly,

$$E_0^{(T)} = \tfrac{1}{2} \operatorname{cth} \tfrac{1}{2}T, \quad \Delta E^{(T)} = \operatorname{th} \tfrac{1}{2}T, \quad G^{(T)}(\tau) = \tfrac{1}{2} \operatorname{cth} \tfrac{1}{2}T(\operatorname{ch} \tau - \operatorname{th} \tfrac{1}{2}T \operatorname{sh} \tau), \tag{9a}$$

$$|\psi_0^{(T)}(X)|^2 = \frac{1}{\sqrt{2\pi \operatorname{sh} T}} \exp\{\tfrac{1}{2}T \operatorname{cth} \tfrac{1}{2}T\} \exp\{-\operatorname{th} \tfrac{1}{2}TX^2\}. \tag{9b}$$

Numerical values of $E_0^{(T)}$, $|\psi_0^{(T)}(X)|^2$, $E_0^{(T,n)}$, for various T, $E_0^{(T,n)}$ obtained using (2) with $m = 1$, are listed in Table 1. We remind that the theoretical values are $E_0 = \frac{1}{2}$, $\Delta E = 1$, $|\psi_0(X)|^2 = (1/\sqrt{\pi}) \exp(-X^2)$, which can be obtained from (9) by taking the limit for $T \to \infty$. It follows from Table 1 that good approximations $E_0^{(T,n)}$ of the theoretical value were achieved at relatively small values of T and n. We cite, for comparison, the results of [3], obtained on a lattice with $N = 51$ partitions and the step $a = 0.5$. The result of exact evaluation of the Gaussian N-dimensional integral is $E_0^{(N)} = 0.447$; the computation of the integral via the simulations of $N_E = 100$ lattice configurations has given the result $E_0^{(N,N_E)} = 0.45$. In paper [2] the result of computations of ($N = 4$)-dimensional integral, obtained in $N_R = 100$ runs each consisting of 10^4 path simulations, is $E_0^{(N,N_R)} = 0.4932 \pm 0.145$; CPU $= 19 \times 100$ s. For $N = 10$, $N_R = 100$ the result is $E_0^{(N,N_R)} = 0.4979 \pm 0.051$; CPU $= 67 \times 100$ s.

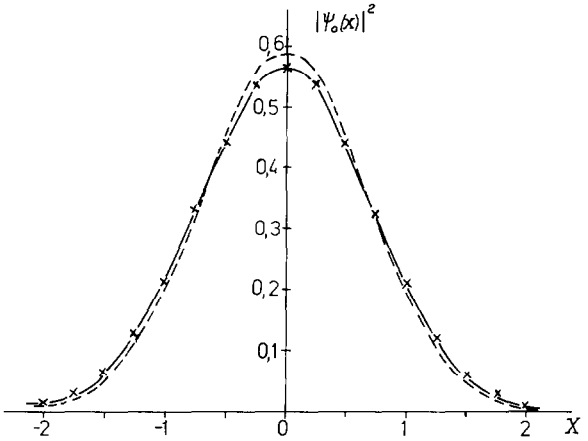

Fig. 1. Wave function of the ground state of harmonic oscillator.

The solid line in Fig. 1 illustrates the theoretical value of $|\psi_0(X)|^2$, the crosses depict our results, obtained via the formula (2) with $m = 1$, $T = 6$, $n = 2$, and the dashed line gives the best result of [3], i.e.

$$|\psi_0^{(N)}(X)|^2 = 0.59 \exp(-1.1X^2) = 1.05 \frac{1}{\sqrt{\pi}} \exp(-1.1X^2),$$

obtained using the exact value of the N-dimensional integral on a lattice with $N = 1000$, $a = 1$ (compare Table 1). We used less than 0.1 s of CPU time at each point X.

Figure 2 is in a logarithmic scale. The crosses represent our values of $G(\tau)$, computed using (2) with $m = 1$, $n = 2$, $T = 6$, CPU time has been within the range of 10 s per point τ. Fitting a straight line (by the method of least squares) we have got $G^{(T,n)}(0) = E_0^{(T,n)} = 0.5053$, $\Delta E^{(T,n)} = -(\mathrm{d}/\mathrm{d}\tau)G^{(T,n)}(\tau) = 1.0198$.

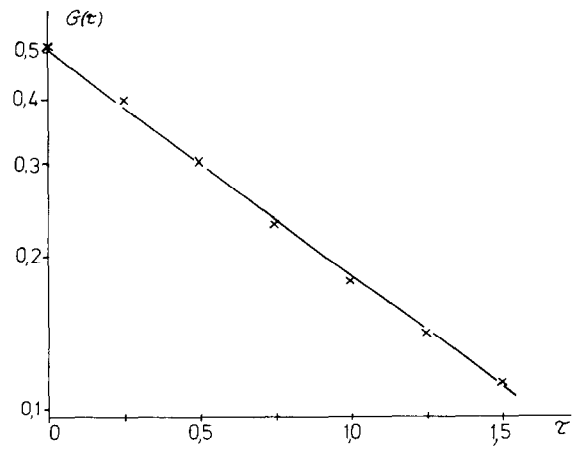

Fig. 2. Dependence of the propagator $G(\tau) = \langle 0 | x(0)x(\tau) | 0 \rangle$ on τ for harmonic oscillator. Its theoretical value is illustrated with the straight line.

Table 2

g	[1] $\check{E}_0$	$N=4$ [2] $G^{(N)}(0)$	$N=20$ [2] $G^{(N)}(0)$	T	Form. (6) $E_0^{(T,1)}$	$G^{(T,1)}(0)$
0.1	0.559146	0.433 ± 0.16	0.409 ± 0.06	3	0.552	0.406
0.2	0.602405	–	–	2.5	0.592	0.364
0.5	0.696176	0.296 ± 0.07	0.293 ± 0.04	2	0.685	0.293
1.0	0.803771	0.269 ± 0.08	0.267 ± 0.08	1.5	0.774	0.257

Table 3

g	[1] $\Delta\check{E}$	[2] $\check{G}(0)$	$N=20$ [2] $\Delta E^{(N)}$	T	Form. (2) $\Delta E^{(T,1)}$	$E_0^{(T,1)}$	$G^{(T,1)}(0)$
0.1	1.2104	0.4125	1.03 ± 0.29	4.5	1.14	0.570	0.419
0.2	1.3481	–	–	4	1.32	0.616	0.377
0.5	1.6282	0.3058	1.50 ± 0.67	3	1.55	0.707	0.313
1.0	1.9341	0.2571	1.56 ± 0.81	2.5	1.88	0.832	0.263

Using the exact value of the integral the authors of the paper [3] have obtained on a lattice with $N = 51$, $a = 0.5$ the value $E^{(N)} = 0.9875$, while when modeling $N_E = 100$ lattice configurations they have got $E^{(N,N_E)} = 0.99$. In [2] the authors have reported

$$E^{(N,N_R)} = 0.8801 \pm 0.202, \quad \text{CPU} = 100 \times 19 \text{ s for } N = 4,$$

$$E^{(N,N_R)} = 0.9331 \pm 0.129, \quad \text{CPU} = 100 \times 67 \text{ s for } N = 10.$$

These values were obtained in $N_R = 100$ runs with 10^4 paths each.

For an inharmonic oscillator our results are obtained using formulae (6) and (2) with $n = m = 1$. The results are listed in Tables 2 and 3. The overall time of computation of $E_0^{(T,1)}$ and $G^{(T,1)}$ has been ca. 0.5 min per point g for the formula (2) and ca. 10 min. per g for (6). Exact values are denoted $\check{E}_0$, $\check{G}(0)$, $\Delta\check{E}$. The results of the paper [2], obtained via 10 simulations of 3000 paths each, are denoted $G^{(N)}(0)$ and $E^{(N)}$. Reported CPU time is 10×25 s per point g for $N = 4$ and 10×17 min. per g for $N = 20$. As $\Delta E^{(T,1)}$ we denote the logarithmic derivative of $G^{(T,1)}(\tau)$ [11], that we find graphically from the points obtained by using (2) with the parameters $n = m = 1$.

All our programs were written in standard Fortran and implemented on the CDC-6500 computer. In [2] the computations were performed on the Vax 780 computer. In [3] this information, as well as on CPU, is not given.

§ 5

Our work in the approximation theory of integration with respect to Gaussian measure is stimulated by the investigations in quantum field theory that are being performed at the Joint Institute for Nuclear Research in Dubna. (Unfortunately, due to limitation of space, we are not able to discuss the results and the wide spectrum of application in detail.) The method of

computation of functional integrals based on the use of conditional Wiener measure and the derived approximation formulae yields the values of the considered quantities with accuracy equal to, and in many cases even with an accuracy greater than, in the Monte Carlo method on lattice, while requiring integrals with essentially lower dimensions. Moreover, our results show, in general, a CPU time shorter by one order. As we have already mentioned at the introduction, we compute these integrals using the quadrature formulas. All these considerations make the 'deterministic approach' an attractive method for the computation of functional integrals.

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